

SEQUENCE LISTING

<110> Beamer, Lesa J.
Eisenberg, David
Carroll, Stephen F.

<120> BACTERICIDAL/PERMEABILITY-INCREASING PROTEIN:
CRYSTALLIZATION, X-RAY DIFFRACTION, THREE-DIMENSIONAL
STRUCTURE DETERMINATION, RATIONAL DRUG DESIGN AND
MOLECULAR MODELING OF RELATED PROTEINS

<130> 11034US02

<140> 09/446,415
<141> 2000-07-19

<150> 08/879,565
<151> 1997-06-20

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<170> PatentIn Ver. 2.1

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Ile	Arg	Glu	Phe	Gln	Leu	Pro	Ser	Ser	Gln	Ile	Ser	Met	Val	Pro	Asn	
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Val	Gly	Leu	Lys	Phe	Ser	Ile	Ser	Asn	Ala	Asn	Ile	Lys	Ile	Ser	Gly	
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Leu	Ser	Ile	Glu	Gly	Met	Ser	Ile	Ser	Ala	Asp	Leu	Lys	Leu	Gly	Ser	
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Asn	Pro	Thr	Ser	Gly	Lys	Pro	Thr	Ile	Thr	Cys	Ser	Ser	Cys	Ser	Ser	
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Leu	Gln	Pro	Tyr	Phe	Gln	Thr	Leu	Pro	Val	Met	Thr	Lys	Ile	Asp	Ser	
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Val	Ala	Gly	Ile	Asn	Tyr	Gly	Leu	Val	Ala	Pro	Pro	Ala	Thr	Thr	Ala	
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Glu	Thr	Leu	Asp	Val	Gln	Met	Lys	Gly	Glu	Phe	Tyr	Ser	Glu	Asn	His	
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Asp Asp Met Ile Pro Lys Glu Ser Lys Phe Arg Leu Thr Thr Lys Phe	
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Phe Gly Thr Phe Leu Pro Glu Val Ala Lys Lys Phe Pro Asn Met Lys	
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Ile Gln Ile His Val Ser Ala Ser Thr Pro Pro His Leu Ser Val Gln	
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Pro Thr Gly Leu Thr Phe Tyr Pro Ala Val Asp Val Gln Ala Phe Ala	
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Val Leu Pro Asn Ser Ser Leu Ala Ser Leu Phe Leu Ile Gly Met His	
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aca act ggt tcc atg gag gtc agc gcc gag tcc aac agg ctt gtt gga	1254
Thr Thr Gly Ser Met Glu Val Ser Ala Glu Ser Asn Arg Leu Val Gly	
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Glu Leu Lys Leu Asp Arg Leu Leu Leu Glu Leu Lys His Ser Asn Ile	
380 385 390	
ggc ccc ttc ccg gtt gaa ttg ctg cag gat atc atg aac tac att gta	1350
Gly Pro Phe Pro Val Glu Leu Leu Gln Asp Ile Met Asn Tyr Ile Val	
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ccc att ctt gtg ctg ccc agg gtt aac gag aaa cta cag aaa ggc ttc	1398
Pro Ile Leu Val Leu Pro Arg Val Asn Glu Lys Leu Gln Lys Gly Phe	
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cct ctc ccg acg ccg gcc aga gtc cag ctc tac aac gta gtg ctt cag	1446
Pro Leu Pro Thr Pro Ala Arg Val Gln Leu Tyr Asn Val Val Leu Gln	
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cct cac cag aac ttc ctg ctg ttc ggt gca gac gtt gtc tat aaa	1491
Pro His Gln Asn Phe Leu Leu Phe Gly Ala Asp Val Val Tyr Lys	
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Asn	Ala	Asn	Ile	Lys	Ile	Ser	Gly	Lys	Trp	Lys	Ala	Gln	Lys	Arg	Phe
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Leu	Lys	Met	Ser	Gly	Asn	Phe	Asp	Leu	Ser	Ile	Glu	Gly	Met	Ser	Ile
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Ile	Glu	Ser	Ala	Leu	Arg	Asn	Lys	Met	Asn	Ser	Gln	Val	Cys	Glu	Lys
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Pro	Val	Met	Thr	Lys	Ile	Asp	Ser	Val	Ala	Gly	Ile	Asn	Tyr	Gly	Leu
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Gly	Glu	Phe	Tyr	Ser	Glu	Asn	His	His	Asn	Pro	Pro	Pro	Phe	Ala	Pro			
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Gly	Val	Leu	Lys	Met	Thr	Leu	Arg	Asp	Asp	Met	Ile	Pro	Lys	Glu	Ser			
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Lys	Phe	Arg	Leu	Thr	Thr	Lys	Phe	Phe	Gly	Thr	Phe	Leu	Pro	Glu	Val			
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Ala	Lys	Lys	Phe	Pro	Asn	Met	Lys	Ile	Gln	Ile	His	Val	Ser	Ala	Ser			
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Thr	Pro	Pro	His	Leu	Ser	Val	Gln	Pro	Thr	Gly	Leu	Thr	Phe	Tyr	Pro			
			325					330					335					
Ala	Val	Asp	Val	Gln	Ala	Phe	Ala	Val	Leu	Pro	Asn	Ser	Ser	Leu	Ala			
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Ser	Leu	Phe	Leu	Ile	Gly	Met	His	Thr	Thr	Gly	Ser	Met	Glu	Val	Ser			
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Asn	Glu	Lys	Leu	Gln	Lys	Gly	Phe	Pro	Leu	Pro	Thr	Pro	Ala	Arg	Val			
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Gln	Leu	Tyr	Asn	Val	Val	Leu	Gln	Pro	His	Gln	Asn	Phe	Leu	Leu	Phe			
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Lys	Ile	Pro	Asp	Tyr	Ser	Asp	Ser	Phe	Lys	Ile	Lys	His	Leu	Gly	Lys	35	40	45	
Gly	His	Tyr	Ser	Phe	Tyr	Ser	Met	Asp	Ile	Arg	Glu	Phe	Gln	Leu	Pro	50	55	60	
Ser	Ser	Gln	Ile	Ser	Met	Val	Pro	Asn	Val	Gly	Leu	Lys	Phe	Ser	Ile	65	70	75	80
Ser	Asn	Ala	Asn	Ile	Lys	Ile	Ser	Gly	Lys	Trp	Lys	Ala	Gln	Lys	Arg	85	90	95	
Phe	Leu	Lys	Met	Ser	Gly	Asn	Phe	Asp	Leu	Ser	Ile	Glu	Gly	Met	Ser	100	105	110	
Ile	Ser	Ala	Asp	Leu	Lys	Leu	Gly	Ser	Asn	Pro	Thr	Ser	Gly	Lys	Pro	115	120	125	
Thr	Ile	Thr	Cys	Ser	Ser	Cys	Ser	Ser	His	Ile	Asn	Ser	Val	His	Val	130	135	140	
His	Ile	Ser	Lys	Ser	Lys	Val	Gly	Trp	Leu	Ile	Gln	Leu	Phe	His	Lys	145	150	155	160
Lys	Ile	Glu	Ser	Ala	Leu	Arg	Asn	Lys	Met	Asn	Ser	Gln	Val	Cys	Glu	165	170	175	
Lys	Val	Thr	Asn	Ser	Val	Ser	Ser	Glu	Leu	Gln	Pro	Tyr	Phe	Gln	Thr	180	185	190	
Leu	Pro	Val	Met	Thr	Lys	Ile	Asp	Ser	Val	Ala	Gly	Ile	Asn	Tyr	Gly	195	200	205	
Leu	Val	Ala	Pro	Pro	Ala	Thr	Thr	Ala	Glu	Thr	Leu	Asp	Val	Gln	Met	210	215	220	
Lys	Gly	Glu	Phe	Tyr	Ser	Glu	Asn	His	His	Asn	Pro	Pro	Pro	Phe	Ala	225	230	235	240
Pro	Pro	Val	Met	Glu	Phe	Pro	Ala	Ala	His	Asp	Arg	Met	Val	Tyr	Leu	245	250	255	
Gly	Leu	Ser	Asp	Tyr	Phe	Phe	Asn	Thr	Ala	Gly	Leu	Val	Tyr	Gln	Glu	260	265	270	
Ala	Gly	Val	Leu	Lys	Met	Thr	Leu	Arg	Asp	Asp	Met	Ile	Pro	Lys	Glu	275	280	285	
Ser	Lys	Phe	Arg	Leu	Thr	Thr	Lys	Phe	Phe	Gly	Thr	Phe	Leu	Pro	Glu	290	295	300	

Val Ala Lys Lys Phe Pro Asn Met Lys Ile Gln Ile His Val Ser Ala
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Ser Thr Pro Pro His Leu Ser Val Gln Pro Thr Gly Leu Thr Phe Tyr
 325 330 335

Pro Ala Val Asp Val Gln Ala Phe Ala Val Leu Pro Asn Ser Ser Leu
 340 345 350

Ala Ser Leu Phe Leu Ile Gly Met His Thr Thr Gly Ser Met Glu Val
 355 360 365

Ser Ala Glu Ser Asn Arg Leu Val Gly Glu Leu Lys Leu Asp Arg Leu
 370 375 380

Leu Leu Glu Leu Lys His Ser Asn Ile Gly Pro Phe Pro Val Glu Leu
 385 390 395 400

Leu Gln Asp Ile Met Asn Tyr Ile Val Pro Ile Leu Val Leu Pro Arg
 405 410 415

Val Asn Glu Lys Leu Gln Lys Gly Phe Pro Leu Pro Thr Pro Ala Arg
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Val Gln Leu Tyr Asn Val Val Leu Gln Pro His Gln Asn Phe Leu Leu
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Phe Gly Ala Asp Val Val Tyr Lys
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 5)

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Thr Leu Pro Asp Phe Thr Gly Asp Leu Arg Ile Pro His Val Gly Arg
 35 40 45

Gly Arg Tyr Glu Phe His Ser Leu Asn Ile His Ser Cys Glu Leu Leu
 50 55 60

His Ser Ala Leu Arg Pro Val Pro Gly Gln Gly Leu Ser Leu Ser Ile
 65 70 75 80

Ser Asp Ser Ser Ile Arg Val Gln Gly Arg Trp Lys Val Arg Lys Ser
 85 90 95

Phe	Phe	Lys	Leu	Gln	Gly	Ser	Phe	Asp	Val	Ser	Val	Lys	Gly	Ile	Ser		
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Ile	Ser	Val	Asn	Leu	Leu	Leu	Gly	Ser	Glu	Ser	Ser	Gly	Arg	Pro	Thr		
		115					120					125					
Val	Thr	Ala	Ser	Ser	Cys	Ser	Ser	Asp	Ile	Ala	Asp	Val	Glu	Val	Asp		
	130					135					140						
Met	Ser	Gly	Asp	Leu	Gly	Trp	Leu	Leu	Asn	Leu	Phe	His	Asn	Gln	Ile		
145					150					155					160		
Glu	Ser	Lys	Phe	Gln	Lys	Val	Leu	Glu	Ser	Arg	Ile	Cys	Glu	Met	Ile		
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Gln	Lys	Ser	Val	Ser	Ser	Asp	Leu	Gln	Pro	Tyr	Leu	Gln	Thr	Leu	Pro		
			180					185					190				
Val	Thr	Thr	Glu	Ile	Asp	Ser	Phe	Ala	Asp	Ile	Asp	Tyr	Ser	Leu	Val		
	195						200					205					
Glu	Ala	Pro	Arg	Ala	Thr	Ala	Gln	Met	Leu	Glu	Val	Met	Phe	Lys	Gly		
	210					215					220						
Glu	Ile	Phe	His	Arg	Asn	His	Arg	Ser	Pro	Val	Thr	Leu	Leu	Ala	Ala		
225					230				235						240		
Val	Met	Ser	Leu	Pro	Glu	Glu	His	Asn	Lys	Met	Val	Tyr	Phe	Ala	Ile		
			245						250					255			
Ser	Asp	Tyr	Val	Phe	Asn	Thr	Ala	Ser	Leu	Val	Tyr	His	Glu	Glu	Gly		
			260					265					270				
Tyr	Leu	Asn	Phe	Ser	Ile	Thr	Asp	Asp	Met	Ile	Pro	Pro	Asp	Ser	Asn		
	275						280				285						
Ile	Arg	Leu	Thr	Thr	Lys	Ser	Phe	Arg	Pro	Phe	Val	Pro	Arg	Leu	Ala		
	290					295					300						
Arg	Leu	Tyr	Pro	Asn	Met	Asn	Leu	Glu	Leu	Gln	Gly	Ser	Val	Pro	Ser		
305					310					315					320		
Ala	Pro	Leu	Leu	Asn	Phe	Ser	Pro	Gly	Asn	Leu	Ser	Val	Asp	Pro	Tyr		
				325					330					335			
Met	Glu	Ile	Asp	Ala	Phe	Val	Leu	Leu	Pro	Ser	Ser	Ser	Lys	Glu	Pro		
			340					345					350				
Val	Phe	Arg	Leu	Ser	Val	Ala	Thr	Asn	Val	Ser	Ala	Thr	Leu	Thr	Phe		
		355					360					365					
Asn	Thr	Ser	Lys	Ile	Thr	Gly	Phe	Leu	Lys	Pro	Gly	Lys	Val	Lys	Val		
	370					375					380						
Glu	Leu	Lys	Glu	Ser	Lys	Val	Gly	Leu	Phe	Asn	Ala	Glu	Leu	Leu	Glu		
385					390					395					400		

Ala Leu Leu Asn Tyr Tyr Ile Leu Asn Thr Phe Tyr Pro Lys Phe Asn
405 410 415

Asp Lys Leu Ala Glu Gly Phe Pro Leu Pro Leu Leu Lys Arg Val Gln
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35 40 45

Ser Glu Val Lys Val Thr Glu Leu Gln Leu Thr Ser Ser Glu Leu Asp
50 55 60

Phe Gln Pro Gln Gln Glu Leu Met Leu Gln Ile Thr Asn Ala Ser Leu
65 70 75 80

Gly Leu Arg Phe Arg Arg Gln Leu Leu Tyr Trp Phe Phe Tyr Asp Gly
85 90 95

Gly Tyr Ile Asn Ala Ser Ala Glu Gly Val Ser Ile Arg Thr Gly Leu
100 105 110

Glu Leu Ser Arg Asp Pro Ala Gly Arg Met Lys Val Ser Asn Val Ser
115 120 125

Cys Gln Ala Ser Val Ser Arg Met His Ala Ala Phe Gly Gly Thr Phe
130 135 140

Lys Lys Val Tyr Asp Phe Leu Ser Thr Phe Ile Thr Ser Gly Met Arg
145 150 155 160

Phe Leu Leu Asn Gln Gln Ile Cys Pro Val Leu Tyr His Ala Gly Thr
165 170 175

Val Leu Leu Asn Ser Leu Leu Asp Thr Val Pro Val Arg Ser Ser Val
180 185 190

Asp	Glu	Leu	Val	Gly	Ile	Asp	Tyr	Ser	Leu	Met	Lys	Asp	Pro	Val	Ala		
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Ser	Thr	Ser	Asn	Leu	Asp	Met	Asp	Phe	Arg	Gly	Ala	Phe	Phe	Pro	Leu		
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225					230					235					240		
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Leu	Val	Gly	Asp	Lys	Val	Pro	His	Asp	Leu	Asp	Met	Leu	Leu	Arg	Ala		
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Thr	Tyr	Phe	Gly	Ser	Ile	Val	Leu	Leu	Ser	Pro	Ala	Val	Ile	Asp	Ser		
	290					295					300						
Pro	Leu	Lys	Leu	Glu	Leu	Arg	Val	Leu	Ala	Pro	Pro	Arg	Cys	Thr	Ile		
305					310					315					320		
Lys	Pro	Ser	Gly	Thr	Thr	Ile	Ser	Val	Thr	Ala	Ser	Val	Thr	Ile	Ala		
				325					330					335			
Leu	Val	Pro	Pro	Asp	Gln	Pro	Glu	Val	Gln	Leu	Ser	Ser	Met	Thr	Met		
			340					345					350				
Asp	Ala	Arg	Leu	Ser	Ala	Lys	Met	Ala	Leu	Arg	Gly	Lys	Ala	Leu	Arg		
		355					360					365					
Thr	Gln	Leu	Asp	Leu	Arg	Arg	Phe	Arg	Ile	Tyr	Ser	Asn	His	Ser	Ala		
	370					375					380						
Leu	Glu	Ser	Leu	Ala	Leu	Ile	Pro	Leu	Gln	Ala	Pro	Leu	Lys	Thr	Met		
385					390					395					400		
Leu	Gln	Ile	Gly	Val	Met	Pro	Met	Leu	Asn	Glu	Arg	Thr	Trp	Arg	Gly		
				405					410					415			
Val	Gln	Ile	Pro	Leu	Pro	Glu	Gly	Ile	Asn	Phe	Val	His	Glu	Val	Val		
			420					425					430				
Thr	Asn	His	Ala	Gly	Phe	Leu	Thr	Ile	Gly	Ala	Asp	Leu	His	Phe	Ala		
	435						440					445					
Lys	Gly	Leu	Arg	Glu	Val	Ile	Glu	Lys	Asn	Arg	Pro	Ala	Asp	Val	Arg		
	450					455					460						
Ala	Ser	Thr	Ala	Pro	Thr	Pro	Ser	Thr	Ala	Ala	Val						
465					470					475							

<210> 6

<211> 470

<212> PRT

<213> Human

<220>

<223> cholesteryl ester transfer protein (CETP) (Figure 5)

<400> 6

His	Glu	Ala	Gly	Ile	Val	Cys	Arg	Ile	Thr	Lys	Pro	Ala	Leu	Leu	Val
1				5					10					15	
Leu	Asn	His	Glu	Thr	Ala	Lys	Val	Ile	Gln	Thr	Ala	Phe	Gln	Arg	Ala
			20					25					30		
Ser	Tyr	Pro	Asp	Ile	Thr	Gly	Glu	Lys	Ala	Met	Met	Leu	Leu	Gly	Gln
		35					40					45			
Val	Lys	Tyr	Gly	Leu	His	Asn	Ile	Gln	Ile	Ser	His	Leu	Ser	Ile	Ala
	50					55					60				
Ser	Ser	Gln	Val	Glu	Leu	Val	Glu	Ala	Lys	Ser	Ile	Asp	Val	Ser	Ile
65					70					75					80
Gln	Asn	Val	Ser	Val	Val	Phe	Lys	Gly	Thr	Leu	Lys	Tyr	Gly	Tyr	Thr
				85					90					95	
Thr	Ala	Trp	Trp	Leu	Gly	Ile	Asp	Gln	Ser	Ile	Asp	Phe	Glu	Ile	Asp
			100					105					110		
Ser	Ala	Ile	Asp	Leu	Gln	Ile	Asn	Thr	Gln	Leu	Thr	Cys	Asp	Ser	Gly
		115					120					125			
Arg	Val	Arg	Thr	Asp	Ala	Pro	Asp	Cys	Tyr	Leu	Ser	Phe	His	Lys	Leu
	130					135					140				
Leu	Leu	His	Leu	Gln	Gly	Glu	Arg	Glu	Pro	Gly	Trp	Ile	Lys	Gln	Leu
145					150					155					160
Phe	Thr	Asn	Phe	Ile	Ser	Phe	Thr	Leu	Lys	Leu	Val	Leu	Lys	Gly	Gln
				165					170					175	
Ile	Cys	Lys	Glu	Ile	Asn	Val	Ile	Ser	Asn	Ile	Met	Ala	Asp	Phe	Val
			180					185					190		
Gln	Thr	Arg	Ala	Ala	Ser	Ile	Leu	Ser	Asp	Gly	Asp	Ile	Gly	Val	Asp
		195					200					205			
Ile	Ser	Leu	Thr	Gly	Asp	Pro	Val	Ile	Thr	Ala	Ser	Tyr	Leu	Glu	Ser
	210					215					220				
His	His	Lys	Gly	His	Phe	Ile	Tyr	Lys	Asn	Val	Ser	Glu	Asp	Leu	Pro
225					230					235					240
Leu	Pro	Thr	Phe	Ser	Pro	Thr	Leu	Leu	Gly	Asp	Ser	Arg	Met	Leu	Tyr
				245					250					255	
Phe	Trp	Phe	Ser	Glu	Arg	Val	Phe	His	Ser	Leu	Ala	Lys	Val	Ala	Phe
			260					265					270		

Gln Asp Gly Arg Leu Met Leu Ser Leu Met Gly Asp Glu Phe Lys Ala
 275 280 285

Val Leu Glu Thr Trp Gly Phe Asn Thr Asn Gln Glu Ile Phe Gln Glu
 290 295 300

Val Val Gly Gly Phe Pro Ser Gln Ala Gln Val Thr Val His Cys Leu
 305 310 315 320

Lys Met Pro Lys Ile Ser Cys Gln Asn Lys Gly Val Val Val Asn Ser
 325 330 335

Ser Val Met Val Lys Phe Leu Phe Pro Arg Pro Asp Gln Gln His Ser
 340 345 350

Val Ala Tyr Thr Phe Glu Glu Asp Ile Val Thr Thr Val Gln Ala Ser
 355 360 365

Tyr Ser Lys Lys Lys Leu Phe Leu Ser Leu Leu Asp Phe Gln Ile Thr
 370 375 380

Pro Lys Thr Val Ser Asn Leu Thr Glu Ser Ser Ser Glu Ser Ile Gln
 385 390 395 400

Ser Phe Leu Gln Ser Met Ile Thr Ala Val Gly Ile Pro Glu Val Met
 405 410 415

Ser Arg Leu Glu Val Val Phe Thr Ala Leu Met Asn Ser Lys Gly Val
 420 425 430

Ser Leu Phe Asp Ile Ile Asn Pro Glu Ile Ile Thr Arg Asp Gly Phe
 435 440 445

Leu Leu Leu Gln Met Asp Phe Gly Phe Pro Glu His Leu Leu Val Asp
 450 455 460

Phe Leu Gln Ser Leu Ser
 465 470

<210> 7
 <211> 24
 <212> DNA
 <213> Human

<220>
 <223> BPI-53

<400> 7
 actggttcca tggaggtcag cgcc

<210> 8
 <211> 29
 <212> DNA
 <213> Human

<220>

<223> BPI-54

<400> 8

gacagatctc tcgagtcatt tatagacaa

29

<210> 9

<211> 42

<212> DNA

<213> Human

<220>

<223> oligonucleotide from XcmI site to SphI site within
BPI gene (encoding residues 348-361) containing
the codon TCC for the serine at amino acid
position 351

<400> 9

cccaactcct ccctggcttc cctcttcctg attggcatgc ac

42

<210> 10

<211> 42

<212> DNA

<213> Human

<220>

<223> Oligonucleotide complementary to SEQ ID NO:5

<400> 10

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42

<210> 11

<211> 14

<212> PRT

<213> Human

<220>

<223> "wild type" amino acid sequence of residues
348-361 in BPI

<400> 11

Pro Asn Ser Ser Leu Ala Ser Leu Phe Leu Ile Gly Met His

1

5

10

<210> 12

<211> 42

<212> DNA

<213> Human

<220>

<223> oligonucleotide from XcmI site to SphI site within
the BPI gene (encoding residues 348-361)
containing the codon GCC for alanine at amino acid
position 351

<400> 12
cccaactccg ccctggcttc cctcttcttg attggcatgc ac 42

<210> 13
<211> 42
<212> DNA
<213> Human

<220>
<223> Oligonucleotide complementary to SEQ ID NO:8

<400> 13
gggttcaggc gggaccgaag ggagaaggac taaccgtacg tg 42

<210> 14
<211> 14
<212> PRT
<213> Human

<220>
<223> "nonglycosylated" amino acid sequence of residues
348-361 in BPI

<400> 14
Pro Asn Ser Ala Leu Ala Ser Leu Phe Leu Ile Gly Met His
1 5 10